Letters to the Editor

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22

STUDY OF LIGHT ABSORPTION IN 8-HYDROXY-1-METHYL QUINOLINIUM HYDROXIDE ANHYDRO-SALT IN STATE OF SOLUTION

S. P TANDON*, K. TANDON** AND J P. SAXENA**

UNIVERSITY OF JODHPUR, JODHPUR, INDIA

(*Received October 1 1966*)

Though the general features of the spectrum of some of the phenol-betaines have been described (Phillips and Keown, 1951; Saxena *et al*, 1959), no systematic study of the characteristics and assignments of their absorption bands has been reported so far. The present communication reports probable assignments for the bands of 8-hydroxy-1-methyl quinolinium hydroxide anhydro-salt, observed in the region 185-600mμ based on characteristics and influence of solvent on them.

Four bands at 18180, 26670, 34480 and 41150 cm^{-1} were recorded with an UVISPEK spectrophotometer in the case of 8-hydroxy-1-methyl quinolinium hydroxide anhydro-salt prepared by the method described by Saxena *et al* (1959) dissolved in chloroform

The intensity (molar extinction coefficient, $\epsilon \sim 10^2$, oscillator strength $f \sim 10^{-3}$) coupled with blue-shift of the 18180 cm^{-1} band $\sim$ 3560 cm^{-1} in changing the solvent from chloroform to ethanol clearly indicates it to be due to a forbidden $n \rightarrow \pi^*$ transition. The n-orbital is presumed to be localised predominantly near phenolic oxygen Hence this transition diminishes electron density near the region of n-orbital. The presence of hydrogen bonds places a positive charge near oxygen atom making it more difficult to remove the electron from the non-bonding orbital. This explains the blue-shift of the band in hydrogen-bonding-solvents (Strickler and Kasha, 1964; Mookherji and Tandon, 1965).

**Chemical laboratories.

*Physical laboratories.

The band at 26670 has intensity ($\epsilon \sim 10^3$; $f \sim 10^{-2}$) suggesting it to be due to an allowed transition. The solvent effect is similar to the 18180 cm^{-1} band. Hence the band may be assigned to an allowed $n \rightarrow \pi^*$ transition.

The bands at 34480 and 41150 cm^{-1} are intense ($\epsilon \sim 10^4$; $f \sim 10^{-1}$) and exhibit typical red shift in solvents of increasing polarity and having large hydrogen bonding power (McConnell, 1952). Hence they may be due to allowed $\pi \rightarrow \pi^*$ transitions.

The study of these bands using polarized light in solid state, and technique of diffuse reflectance in powder state is in progress. An attempt is also being made to evaluate the various molecular orbitals involved.

The authors wish to thank Prof. R. C Kapoor, Head of the Chemistry Department for providing the facilities for the work

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